

Experimental and Simulated Solubilities of Gases in Dialkylimidazolium Ionic Liquids

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Solubility measurements can constitute an important source of information about the structure and molecular interactions in solution. In this work, solubility experiments are associated to free energy calculations by computer simulation to model phase equilibria and to calculate gas solubilities in ionic liquids.

The solubility of several gases (oxygen, carbon dioxide, methane, argon) in butyl methyl imidazolium based ionic liquids (namely [bmim][BF₄] and [bmim][PF₆]) was measured using an isochoric saturation method in which the quantity of dissolved gas is determined from the measurement of the equilibrium pressure of the saturated solution produced by the contact of known amounts of dry gas and degassed solvent. The solubility can be expressed in terms of Henry's law coefficients and from there, the standard Gibbs energy of solvation is calculated. The standard enthalpy of solvation is derived from the variation of the Henry's law coefficients with temperature.

New force fields for dialkylimidazolium-based ionic liquids were formulated from quantum mechanical calculations associated with molecular dynamic simulations. Standard Gibbs energies of solvation were calculated. The Henry's law coefficients obtained from the simulation results are compared with experimental values and structural details of the solution are investigated.